STRUCTURE AND ELECTRONIC PROPERTIES OF NOVEL UNCONVENTIONAL CARBON ALLOTROPES AND BN POLYMORPHES

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Unconventional allotropic modifications of carbon and polymorphic phases of boron nitride known in the literature are survived, including amorphic and metallic carbon, carbon C8, carbynes, nanotubular crystals, "cubic graphite", chaoites, E-phase, etc. Their structures predicted theoretically and found experimentally are collected, and analyzed critically.

Full set of fullerene clusters (molecules) as building units of close packed crystals was predicted theoretically. Elementary cells of face centered, body centered cubic, hexagonal, diamond and other lattices were designed.

Energy band structure, the equation of states, the densities of electronic states. and the electronic density map of novel allotropic modifications of carbon and polymorphes of BN have been calculated in first time by ab-initio FLAPW method.

Electronic structure of simple cubic fullerites SCF-C24 and fulborenite SCF-B12N12 shown in figure 1 have been calculated. The equilibrium interatomic distance aCC=0.1550 nm and aBN=0.1537 nm is intermediate between diamond (sphalerite) and graphite (h-BN). Band structure consists of 4 (6) filled bands with gap ~1.9 eV and ~0.1 eV respectively. The SCF-C24 was shown to be the diamond-like molecular semiconductor combining the nonpolarisability and porosity with the mechanical strength (bulk module B=308 GPa), chemical inertness, thermal stability and high thermal conductivity. All of these point on the SCF-C24 as the perspective low-dielectric material ($\varepsilon < 5.7$) for interconnectors and substrates for integrated circuits. The SCF-B12N12 was shown to be the diamond-like molecular semimetal.

Electronic structure of fulborenite SCF-B24N24 (fig.1) have been calculated. Its building units clusters B24N24 have been discovered recently in mass-spectra of arc-melting BN. Calculated parameters are: the equilibrium lattice parameter A=0.73458 nm, length of B-N bond aBN=0.1521 nm, number of atoms per unit cell Z=48, density ρ=2.495 g/sm3, bulk module B0= 367 GPa, band gap ΔEg=3.76 eV. It was concluded to be the heteropolar semiconductor or dielectric with specific bulk module higher then for cubic boron nitride.

Electronic structure of hyperdiamond fulborenite HDF-B12N12 (fig.1) have been calculated. Bulk module of HDF-B12N12 B=590 GPa is greater then for diamond (B=540 GPa). This novel boron nitride faujasite type polymorphe is expected to become an extremely super-hard semiconductor.

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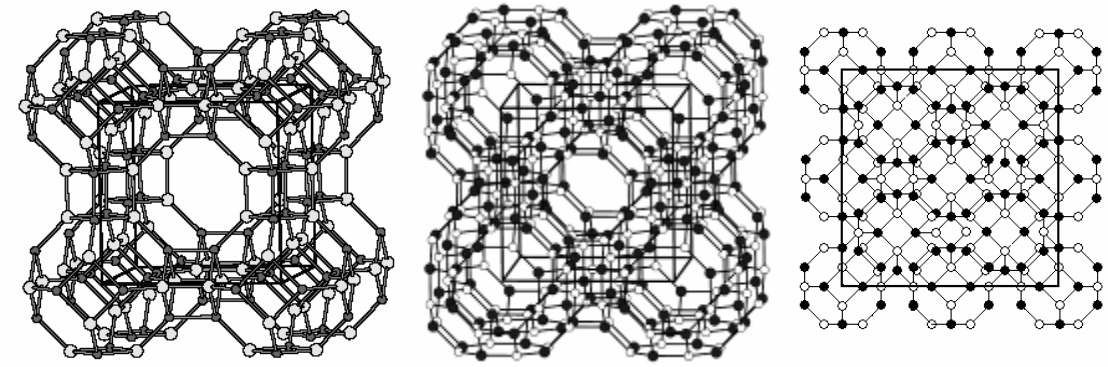

Fig. 1. Elementary cells of the simple cubic fulborenites SCF- $B_{12}N_{12}$ in which molecules $B_{12}N_{12}$ are covalently bonded by square faces, the SCF-$B_{24}N_{24}$ with molecules $B_{24}N_{24}$ bonded by octahedral faces, and hyperdiamonf fulborenite HDF-$B_{12}N_{12}$ with molecules $B_{12}N_{12}$ copolymerized by hexagonal faces.